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MODELING OF TURBULENT MIXING AT DENSITY DISCONTINUITIES IN NONSTEADY COMPRESSIBLE FLOWS

R. I. Issa

R & D Associates
Marina del Rey, CA 90291

September 1981

Final Report

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AIR FORCE WEAPONS LABORATORY
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Kirtland Air Force Base, NM 87117

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This document describes a theoretical modeling of turbulent mixing at density discontinuities in nonsteady compressible flows. It is shown that when density and pressure gradients are large and have opposite signs (e.g., near the combustion products/air contact surface in blast waves driven by high-explosive sources), flow perturbations will be amplified, leading to local turbulent mixing. The applicability of using a turbulence model to simulate this process is examined. The conservation laws (for mass, momentum, energy and species) are presented in mass-averaged form, and the k-ε model of turbulence is applied.

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20. ABSTRACT (Continued)

The relevant term for the generation of turbulent kinetic energy, the term of dominant importance in this problem, is derived by two independent approaches. This generation term is driven by gradients of pressure and density normal to the interface between the high-explosive products of combustion and the shocked air, and not by shear. The present work is thought to represent the first description of a turbulence model for flows driven by such normal gradients.

PREFACE

The author acknowledges the contributions to this work made by Dr. A. L. Kuhl and H. J. Carpenter (both of RDA). They made important contributions to the formulation of the problem and provided physical examples of mixing during the expansion of high explosive charges detonated in air. The manuscript was typed by Ms. J. MacNeish and edited by Dr. Kuhl. Their help is greatly appreciated.

Dr. M. A. Plamondon was the AFWL contact for this project. The results can be used for modeling afterburning in hydrocode calculations of HE blast flows.

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I. INTRODUCTION

1. STATEMENT OF THE PROBLEM

This document describes the theoretical modeling of turbulent mixing at density discontinuities in nonsteady compressible flows. It is well known that if a density discontinuity (or a strong density gradient) occurs in a pressure gradient of the opposite sign, then the flow field is hydrodynamically unstable in the Rayleigh-Taylor sense (Ref. 1). Small perturbations occurring in such a region will amplify with time, and if the perturbations become large enough, they can lead to a local breakdown in the well-ordered flow; i.e., they can lead to turbulence.

One of the more interesting examples of density gradients working against pressure gradients to cause instabilities occurs in blast waves driven by solid high explosives (HE).* After the detonation wave breaks out of the charge, the HE combustion gases expand to a high velocity ($\sim$6 km/s), pushing an air shock ahead. One-dimensional inviscid calculations of this problem (e.g., Ref. 2) show that a positive pressure gradient is formed throughout the flow field. Such calculations also indicate that there is a large density jump (ρ_{HE}/ρ_{air} can be as large as 70) across the contact surface. However, high-speed photography of HE experiments shows that this contact surface (which theoretically should be smooth) actually develops an irregular shape indicating the growth of instabilities. Evidence of mixing at the contact surface can be inferred from test results which show that the HE gases react with the shocked ambient gases and release heat

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*Similar gradients can occur in "shock-tube-type" flows driven by gases at very large initial densities and across progressing flame fronts (i.e., deflagration waves).

(i.e., afterburn) if the ambient gases contain oxygen (Refs. 3,4). Since this heat release can be of the same order as the energy released by the detonation wave (e.g., TNT postdetonation energy release is about 2.5 times the detonation energy), it will affect the blast wave flow field and must be taken into account for accurate numerical simulations of such flows.

This report describes the modeling of such mixing phenomena by the use of a k-ε turbulence model. The fundamental idea is to generate turbulent kinetic energy according to the above-described Rayleigh-Taylor mechanism, which will then produce turbulent mixing in the region of the contact surface. Note that this turbulence mechanism is driven at least initially by pressure and density gradients normal to the contact surface, and not by shear. Turbulence models based on such normal gradients have not been published previously. This report describes the development of the k-ε model and presents closures for the terms arising in such variable density flows.

2. COMMENTS ON FLOW STABILITY

Flow instabilities generate and sustain turbulence (Ref. 5). The following elementary argument is used to identify the origin of an instability in the present flow situation, which can lead to the outbreak of turbulence. It should be stressed, however, that these arguments are of a qualitative nature and do not lead in any way to a quantitative model for the prediction of the time-evolution of the flow.

First, a definition of instability is loosely given here as that condition under which a perturbation in the state of a medium of fluids in equilibrium (or quasi-equilibrium) results in a departure from the state of equilibrium larger than the driving perturbation. Consider now two fluids of densities ρ_A and ρ_B ($\rho_A > \rho_B$) in a state of quasi-equilibrium and subject to a pressure gradient in the direction normal to the interface. The theorem of Bjerknes (Ref. 5) states that the rate of generation of circulation Γ (a measure of vorticity) is given by

$$\frac{d\Gamma}{dt} = -\oint \frac{1}{\rho} \nabla p \cdot d\underline{\ell} \qquad (1)$$

where the integral is taken over a closed contour. Consider an integration path 1-2-3-4 in Figure 1 that encloses a finite portion of the interface separating the two fluids, and where points 2 and 3 and points 1 and 4 are arbitrarily close but straddle the surface. Eq. (1) then yields

$$\frac{d\Gamma}{dt} = -\frac{1}{\rho_A}(p_2-p_1) - \frac{1}{\bar{\rho}}(p_3-p_2) - \frac{1}{\rho_B}(p_4-p_3) - \frac{1}{\bar{\rho}}(p_1-p_4) \qquad (2)$$

where $\bar{\rho}$ is some average density across the interface and $\rho_A > \bar{\rho} > \rho_B$. Since the fluids are in a state of equilibrium and there is no pressure gradient tangential to the interface, then

$$p_1 = p_2 = p_3 = p_4$$

and Eq. (2) reads

$$\frac{d\Gamma}{dt} = 0$$

Thus, no vorticity is generated and the flow retains its equilibrium.

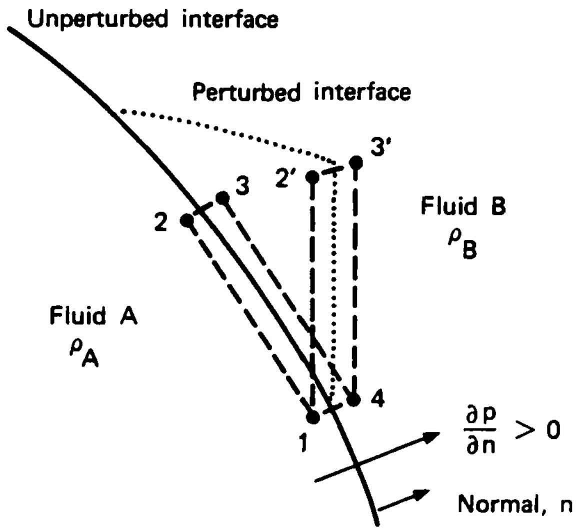

Figure 1. Description of integration paths of Eq. (1) for perturbed and unperturbed interfaces.

Consider now a perturbation in the position of the interface such that points 2 and 3 are removed to new locations 2' and 3'. A pressure gradient tangential to the interface is now set up; Eq. (2) then reads

$$\frac{d\Gamma}{dt} = - \frac{1}{\rho_A}(p_{2'}-p_1) - \frac{1}{\bar{\rho}}(p_{3'}-p_{2'}) - \frac{1}{\rho_B}(p_4-p_{3'}) - \frac{1}{\bar{\rho}}(p_1-p_4)$$

But $p_1 = p_4 = p_2$ and $p_{2'} = p_{3'}$; hence,

$$\frac{d\Gamma}{dt} = \left(\frac{1}{\rho_B} - \frac{1}{\rho_A}\right)(p_{2'}-p_2)$$

For the case when $\rho_A > \rho_B$,

$$\frac{d\Gamma}{dt} = \text{const.} \times \frac{\partial p}{\partial s}$$

In this case the constant is positive, and $\partial p/\partial s$ is the pressure gradient normal to the unperturbed interface. When $\partial p/\partial s$ is positive, a positive circulation is generated which tends to distort the interface further--an unstable situation. Conversely, when $\partial p/\partial s$ is negative, a negative circulation is generated which tends to restore the interface towards its equilibrium state--a stable situation. The flow being considered in the present report corresponds to the positive pressure gradient case with $\rho_A > \rho_B$, and hence it appears to contain inherent instabilities. It will be shown later with a totally different approach that this mechanism (a pressure gradient acting in a variable density flow field) is one of the sources of turbulence generation.

3. ON THE APPLICABILITY OF TURBULENCE MODELING

In the preceding section it was demonstrated that flow instabilities can arise in the problem under consideration. What is not clear, however, is how such instabilities evolve once they have developed and whether they lead to the transition to full turbulence in the normally accepted sense (Ref. 6). In the absence of detailed experimental data, doubts must arise about the validity of classifying the breakdown phenomenon at the interface as turbulence. These doubts are enforced when it is remembered that the macroscopic flow field evolves so rapidly that the time scale of turbulence fluctuations becomes similar to the macroscopic time scale. The applicability of turbulence modeling thus becomes harder to justify.

On the other hand, turbulence can be viewed as a random motion subject to statistical laws; i.e., that the random motion leads to rapid mixing and property exchange. Since it was found experimentally that very rapid mixing occurs in the present flow case, it can be presumed that such a random statistical motion is present. Turbulence modeling endeavors to simulate the exchange processes occurring in this random motion on a macroscopic scale; its applicability to the present case can therefore be justified on these grounds. However, this argument cannot be regarded as conclusive until it is supported either by experiment or by analysis of the microscopic scale motion--tasks that are beyond the present effort.

4. CHOICE OF TURBULENCE MODEL

It is assumed here that the reader is familiar with turbulence modeling; those who are not can find exhaustive discussions on turbulence and its modeling in may texts, such as References 6 through 9.

Most turbulence models were originally developed for the special case of constant density shear flows. A comprehensive review of these models and their closures is given in Reference 9. These standard models contain a manifold of fluctuation correlation terms that require closure.

Models developed for compressible shear flows are based on two types of ensemble averaging. The first is the usual Reynolds averaging, which results in many terms involving density fluctuation, each requiring closure. Models based on this type of averaging will inevitably be complex. An example of a model that utilizes the Reynolds averaging procedure can be found in Reference 10. In that treatment, many simplifications and restrictions pertaining to the atmospheric boundary layer were introduced at the outset which greatly simplified the model. The second approach is the mass-weighted averaging due to Favre (Ref. 11). It results in fewer terms at the expense of clarity of physical interpretation of the averaged variables. Examples of models that are based on mass-weighted averaging can be found in References 12 and 13.

Although the k-ε model (Refs. 7,14) was developed for incompressible flow, there is no objection in principle to its generalization to flows with variable density as was done in Reference 15 with the aid of mass-weighted averaging. All that is required is to devise model closures for the compressible flow terms. The model in its incompressible form has been extensively used over a very wide range of flow problems and has proved to yield reliable predictions in many different flow situations. It was applied in its compressible form as used in Reference 16 to the calculation of supersonic flow with imbedded shocks. With all these considerations taken into account, the k-ε model appears the most attractive model of the alternatives.*

It is felt that none of the existing compressible flow models deals adequately with the "enthalpic" generation term of turbulent kinetic energy, which is regarded in the present case as the main generator of turbulence. In these models attention has been focused on the "kinetic" generation due to stresses and strains rather than the enthalpic generation due to density variations in a pressure gradient field which is of major relevance here. Therefore, the main objective of this document is to devise a suitable closure model for this all-important term.

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*More sophisticated models which solve for the turbulent fluxes were not seriously considered here because of economic considerations. Experience shows that they yield moderate improvement in predictions at a great cost. However, they should not be ruled out for future considerations.

II. ANALYSIS

1. THERMODYNAMIC RELATIONS

The following analysis includes the presence of up to three species of fluids; the generalization to a system consisting of more species is a straightforward extension of what is presented. Different fluids will be labeled with subscripts A, B, and C, having mass m_A, m_B, and m_C, respectively. The mass of the mixture m is then given by

$$m = m_A + m_B + m_C \tag{3}$$

The mixture fractions f_A, f_B and f_C are defined as

$$f_A = \frac{m_A}{m}$$
$$f_B = \frac{m_B}{m}$$
$$f_C = \frac{m_C}{m} \tag{4}$$

From Eqs. (3) and (4) it is clear that

$$f_A + f_B + f_C = 1 \tag{5}$$

If ρ_A, ρ_B, and ρ_C are the densities of the species A, B, and C at the <u>mixture</u> pressure p and temperature T and if ρ is the density of the mixture, then by the law of additive volumes (Ref. 17), one obtains the following:

$$V = V_A(p,T) + V_B(p,T) + V_C(p,T)$$

Hence,

$$\frac{m}{\rho} = \frac{m_A}{\rho_A} + \frac{m_B}{\rho_B} + \frac{m_C}{\rho_C}$$

The last relation can be rewritten with the aid of Eq. (4) as

$$\frac{1}{\rho} = \frac{f_A}{\rho_A} + \frac{f_B}{\rho_B} + \frac{f_C}{\rho_C} \qquad (6)$$

Compressibility Relations

When the fluids are compressible, the following relations may be invoked:

$$\rho_A = \frac{p}{R_A T}$$

$$\rho_B = \frac{p}{R_B T}$$

$$\rho_C = \frac{p}{R_C T} \qquad (7)$$

where it has been assumed that the fluids act as perfect gases with gas contants R_A, R_B, and R_C. The assumption of perfect gas behavior is not a prerequisite and may be replaced by other relations if required. The mixture gas contant R is given by the mass-weighted average

$$R = f_A R_A + f_B R_B + f_C R_C \qquad (8)$$

Similar relations hold for the specific heat quantities C_p and C_v. Combination of Eqs. (6), (7), and (8) yields

$$\rho = \frac{p}{RT} \qquad (9)$$

2. THE TRANSPORT EQUATIONS IN MASS-AVERAGED FORM

As stated earlier, the procedure for mass-averaging was introduced in Reference 11 to simplify considerably the resulting equations and to eliminate a great many of the terms involving density-fluctuation calculations. The basic definitions are now presented, and the transport equations of interest are then stated.

Let the instantaneous value of a dependent variable ϕ be composed of two components: a mean value $\tilde{\phi}$ (where $\sim$ denotes mass-averaging) and a fluctuating component, ϕ'. Thus,

$$\phi = \tilde{\phi} + \phi'$$

The mass-averaged quantity $\tilde{\phi}$ is defined by

$$\tilde{\phi} = \frac{\overline{\rho\phi}}{\bar{\rho}} \tag{10}$$

where the overbar denotes ensemble averaging (Refs. 11,15). ϕ may stand for any variable except p and ρ for which the Reynolds averages are used. Thus,

$$\bar{p} = \overline{\bar{p} + p'}$$

and

$$\bar{\rho} = \overline{\bar{\rho} + \rho'}$$

It follows that

$$\overline{\rho\phi'} = 0 \tag{11}$$

and that

$$\overline{\phi'} = - \frac{\overline{\rho'\phi'}}{\bar{\rho}} \neq 0 \tag{12}$$

The transport equations for mass, momentum, and energy of the mixture in conjunction with the transport equations for the mass fraction can be written in mass-averaged form in Cartesian tensor notation as follows:

<u>Continuity</u>

$$\frac{\partial}{\partial t}\bar{\rho} + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j) = 0 \tag{13}$$

<u>Momentum</u>

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{u}_i) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j\tilde{u}_i) = \frac{\partial}{\partial x_j}\left(-\bar{p}\delta_{ij} + \bar{\tau}_{ij} - \overline{\rho u_i' u_j'}\right) \tag{14}$$

where

$$\tau_{ij} \equiv \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\,\delta_{ij}\,\frac{\partial u_k}{\partial x_k}\right) \tag{15}$$

and μ is the molecular viscosity.

<u>Energy</u>

$$\frac{\partial}{\partial t}(\overline{\rho\tilde{E}}) + \frac{\partial}{\partial x_j}\,\tilde{u}_j\,(\bar{\rho}\tilde{E}+\bar{p}) = \frac{\partial}{\partial x_j}\left(\frac{\mu}{\sigma_h}\,\frac{\partial\tilde{h}}{\partial x_j} - \overline{\rho u'h'}\right)$$

$$+ \frac{\partial}{\partial x_j}\left[\tilde{u}_i(\bar{\tau}_{ij} - \overline{\rho u_i' u_j'}) + \overline{u_i'(\tau_{ij} - \tfrac{1}{2}\rho u_i' u_j')}\right] + \tilde{Q} \tag{16}$$

where $\tilde{E}$ is the mass-averaged total energy, h is the specific enthalpy, σ_h is the Prandtl number for molecular heat diffusion, and Q is the external source of energy (heat of reaction when present). The instantaneous total energy is given by

$$E = e + \frac{1}{2} u_i u_i$$

where e is the specific internal energy. Taking the mass-weighted ensemble average of the above relation gives

$$\tilde{E} = \tilde{e} + \frac{1}{2} \tilde{u}_i \tilde{u}_i + \frac{1}{2} \frac{\overline{\rho u_i' u_i'}}{\bar{\rho}}$$

where the last term is the average kinetic energy of turbulence, k. The last expression can then be written as

$$\tilde{E} = \tilde{e} + \frac{1}{2} \tilde{u}_i \tilde{u}_i + k \tag{17}$$

<u>Mass Fraction</u>

$$\frac{\partial}{\partial t} \bar{\rho} \tilde{f}_\alpha + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_j \tilde{f}_\alpha) = \frac{\partial}{\partial x_j} \left[\frac{\mu}{\sigma_\alpha} \frac{\partial \tilde{f}_\alpha}{\partial x_j} - \overline{\rho u_j' f_\alpha'} \right] + S_\alpha \tag{18}$$

where subscript α denotes the species (A, B or C), σ_α is the Prandtl number for the molecular diffusion of fluid component α, and S_α is the source or sink of component α (due to chemical reaction, for example).

Also needed is the equation for the transport of turbulent kinetic energy k, which is as follows:

Turbulent Kinetic Energy

$$\frac{\partial}{\partial t}\bar{\rho}k + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j k) = \frac{\partial}{\partial x_j}\left(\overline{\tau_{ij}u_i'} - \overline{\rho u_i' k} - \overline{u_i' p_i'}\right)$$

$$- \overline{\rho u_i' u_j'}\,\frac{\partial}{\partial x_j}\,\tilde{u}_i - \overline{u_i'}\,\frac{\partial}{\partial x_i}\,\bar{p} - \overline{p'\frac{\partial u_i'}{\partial x_i}} - \overline{\tau_{ij}\frac{\partial u_i'}{\partial x_j}} \qquad (19)$$

It should be noted that the preceding transport equations are exact insofar as the original instantaneous equation from which they are derived is exact. For flows without fluctuations, all the (') quantities vanish and the equations reduce to their laminar forms. The significance of the terms involving fluctuation correlations in Eqs. (14) to (19) is discussed and explained in the many existing texts on turbulence such as References 6-9, 11, and 15. The most notable of the correlation terms are those of the form $\overline{\rho u_i' \phi}$ where ϕ may stand for any of the dependent variables. These terms are <u>universally</u> regarded as representing the turbulent fluxes of property ϕ. The aim in turbulence modeling is to provide the most accurate and universal representations of these terms, which is called turbulence model closure.

A significant difference between the compressible and the incompressible equations is the presence of two extra terms, $-\overline{u_i'}(\partial\bar{p}/\partial x_i)$ and $-\overline{p'(\partial u_i'/\partial x_i)}$; in the former case, both terms can be regarded as turbulent energy generation terms. It will be seen later that the first of these terms plays the all-important role in the present flow problem.

3. THE k-ε MODEL

The k-ε model (Ref. 7) employs the hypothesis of eddy diffusivity for the evaluation of the turbulent exchange processes. Thus, for any turbulent flux $-\overline{\rho u_i' \phi}$ for scalar property ϕ, the expression is replaced by

$$-\overline{\rho u_i'\phi'} \equiv \frac{\mu_t}{\sigma_{t,\phi}} \frac{\partial\tilde{\phi}}{\partial x_i} \tag{20}$$

where μ_t is the eddy viscosity to be defined later and $\sigma_{t,\phi}$ is the turbulence Prandtl number for the diffusion of scalar property ϕ. For the turbulent exchange of momentum, the turbulent flux is represented by

$$-\overline{\rho u_i'u_j'} \equiv \mu_t\varepsilon_{ij} - \frac{2}{3}\ \delta_{ij}k\bar{\rho} \tag{21}$$

where

$$\varepsilon_{ij} \equiv \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\ \delta_{ij}\frac{\partial\tilde{u}_k}{\partial x_k} \tag{22}$$

Thus, many of the correlation terms are replaced by terms involving gradients of the mean quantities. There remain still a few correlation terms that require closure; they are dealt with now, one by one.

The term $-1/2[\overline{u_i'(\rho u_i'u_i')}]$ in the energy Eq. (16) is almost the same as $-\overline{\rho u_j'k}$ which is as already discussed, the turbulent flux of k. Hence, the term may be replaced by the following:

$$-\frac{1}{2}\ \overline{u_i'\rho u_i'u_j'} \equiv \frac{\mu_t}{\sigma_{t,k}} \frac{\partial k}{\partial x_j} \tag{23}$$

The terms $\partial/\partial x_j(\overline{\tau_{ij}u_i'} - \overline{u_i'p'})$ in Eq. (19) are normally regarded as diffusion ones and are lumped with $-\overline{\rho u_j'k}$. Also in Eq. (19) the terms $-u_i'(\partial\bar{p}/\partial x_i) - p'(\partial u_i'/\partial x_i)$ require closure. These are regarded as generation terms arising from the variations in density; they warrant special attention for this problem and are therefore dealt with in a separate section. For the moment, however, they will be lumped with the kinetic generation term to give the total generation term G as

$$G = -\overline{\rho u_i' u_j'} \frac{\partial \tilde{u}_i}{\partial x_j} - \overline{u_i'} \frac{\partial \bar{p}}{\partial x_i} - \overline{p' \frac{\partial u_i'}{\partial x_i}} \tag{24}$$

Finally, the term $\overline{\tau_{ij}(\partial u_i'/\partial x_j)}$ is regarded as the dissipation rate per unit mass of the turbulent energy and is represented by a new variable ε which is the volumetric dissipation rate of turbulent energy. Hence,

$$\overline{\tau_{ij} \frac{\partial u_i'}{\partial x_j}} \equiv \bar{\rho}\varepsilon \tag{25}$$

The variable ε must now be determined. To this end, a transport equation for ε is formulated and solved in conjunction with the rest of the transport equations. This equation takes a form similar to that for k in Eq. (19), and is given by Reference 8.

$$\frac{\partial}{\partial t} \bar{\rho}\varepsilon + \frac{\partial}{\partial x_j} (\bar{\rho}\tilde{u}_j \varepsilon) = \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_{t,\varepsilon}} \frac{\partial \varepsilon}{\partial x_j} \right) + C_1 G\varepsilon/k + C_2 \rho\varepsilon^2/k \tag{26}$$

where C_1 and C_2 are empirical constants.

It remains to determine the eddy viscosity μ_t, which is evaluated from

$$\mu_t \equiv C_\mu \bar{\rho} k^2/\varepsilon \tag{27}$$

where C_μ is another empirical constant.

The model is now closed except for the enthalpic generation terms in Eq. (24) which are dealt with in the following section.

4. CLOSURE FOR ENTHALPIC GENERATION

The generation G of turbulent kinetic energy is given by Eq. (24) as:

$$G = -\overline{\rho u_i' u_j'} \frac{\partial \tilde{u}_i}{\partial x_j} - \overline{u_i'} \frac{\partial \bar{p}}{\partial x_i} - \overline{p' \frac{\partial u_i'}{\partial x_i}}$$

The first term in the expression is the kinetic production term due to work by turbulent stresses acting in a strain field; the closure for the turbulent stresses is given by Eqs. (21) and (22). The remaining two terms in the expression for G are the enthalpic generation due to the work of fluctuating mass-velocity against a pressure gradient and the work of fluctuating pressure against a fluctuating strain field, respectively.

For the problem under consideration, the pressure gradient is considerable and the density fluctuations are very large at the interface because of the high-density gradient across it. The term $-\overline{u_i'}(\partial\bar{p}/\partial x_i)$ is, therefore, expected to be a major contributor to the generation of turbulence at the interface. On the other hand, the pressure fluctuations are not thought to be very large, and smaller still will be the strain fluctuations $\partial u_i'/\partial x_i$. The term $\overline{p'(\partial u_i'/\partial x_i)}$ may in this case be neglected in comparison to the previous term.*

*The term $p'(\overline{\partial u_i'/\partial x_i})$ was analyzed as a diffusion term in Reference 18 and not as a generation term. It is not clear how this conclusion was reached as no justification was given.

The task now is to provide a closure for the term $-\overline{u_i'}(\partial\bar{p}/\partial x_i)$, which may be rewritten with the aid of relation Eq. (12) as $(\overline{\rho' u_i'}/\bar{\rho})(\partial\bar{p}/\partial x_i)$. In what follows, two independent paths are taken to obtain such closure; it will be shown that the resulting closures are almost equivalent.

a. First approach--To arrive at an expression for the correlation $\overline{\rho' u_i'}$, one may use the arguments presented in Reference 19. Since mass-weighted averaging is employed presently, the derivation below is a slight modification of the one presented in that reference.

The density fluctuation may be written in terms of mass-weighted quantities as

$$\rho' = -\frac{L}{\sqrt{k}}\,\frac{\rho u_j'}{\bar{\rho}}\,\frac{\partial\bar{\rho}}{\partial x_j} \tag{28}$$

where L is a length scale. When Eq. (28) is multiplied by u_i' and then ensemble-averaged, the following relation is obtained:

$$\overline{\rho' u_i'} = -\frac{L}{\sqrt{k}}\,\frac{\overline{\rho u_i' u_j'}}{\bar{\rho}}\,\frac{\partial\bar{\rho}}{\partial x_j} \tag{29}$$

Now L is given in Reference 20 as

$$L \approx C_3\,\frac{\mu_t}{\frac{2}{3}\sqrt{k}\,\bar{\rho}} \tag{30}$$

and $-\overline{\rho u_i' u_j'}$ is here modeled by Eq. (21). Hence,

$$\overline{\rho' u_i'} = -C_3\,\frac{\mu_t}{\bar{\rho}}\,\delta_{ij}\,\frac{\partial\bar{\rho}}{\partial x_j} + \frac{3}{2}\,C_3\,\frac{\mu_t^2}{\bar{\rho}^2 k}\,\varepsilon_{ij}\,\frac{\partial\bar{\rho}}{\partial x_j}$$

where C_3 is another empirical constant. The enthalpic generation term thus becomes

$$-\overline{u_i'}\,\frac{\partial\bar{p}}{\partial x_i} = -\frac{C_3\mu_t}{\bar{\rho}^2}\left[\delta_{ij} - \frac{3}{2}\frac{\mu_t}{\bar{\rho}k}\,\varepsilon_{ij}\right]\frac{\partial\bar{\rho}}{\partial x_j}\,\frac{\partial\bar{p}}{\partial x_i} \qquad (31)$$

When $\partial\bar{\rho}/\partial x_i$ is negative and $\partial\bar{p}/\partial x_i$ is positive, as is the present case, for i=j the term in the square bracket is almost certain to be positive since the normal strain field is small; hence, the generation term gives a positive contribution. For the case when the sign of either $\partial\bar{p}/\partial x_i$ or $\partial\bar{\rho}/\partial x_i$ is reversed, the term reverses its role and acts to destroy turbulence energy. The action of the term does, therefore, follow the trends already discussed in Section I-2.

b. Second approach--In the second approach, the density fluctuation is obtained from an equation that relates the density to other dependent variables; Eq. (6) serves this purpose. A displacement ρ' is considered to result in a displacement in all other variables such that the ensemble average of fluctuations in mass-weighted terms vanishes. Thus, ρ' results in displacement $\rho f_\alpha'/\bar{\rho}$ and $\rho T'/\bar{\rho}$ and so on. Eq. (6) then gives

$$-\frac{\rho'}{\bar{\rho}^2} = \frac{\rho}{\bar{\rho}}\left(\frac{f_A'}{\bar{\rho}_A} + \frac{f_B'}{\bar{\rho}_B} + \frac{f_C'}{\bar{\rho}_C}\right) - \left(\frac{\rho_A'\tilde{f}_A}{\bar{\rho}_A^2} + \frac{\rho_B'\tilde{f}_B}{\bar{\rho}_B^2} + \frac{\rho_C'\tilde{f}_C}{\bar{\rho}_C^2}\right) \qquad (32)$$

It should be noted that the first term on the right-hand side of Eq. (32) is due to the variations in density regardless of the effects of compressibility; it is present even if the flow is incompressible. The second term expresses the effects of compressibility of the different gas components.

From Eq. (7) the fluctuations ρ_A', ρ_B' and ρ_C' may be obtained in terms of fluctuations in T and p. Thus,

$$\frac{\rho_\alpha'}{\bar{\rho}_\alpha} = \frac{p'}{\bar{p}} - \frac{\rho T'}{\bar{\rho}\tilde{T}} \tag{33}$$

where α stands for A, B and C.

Substitution of Eq. (33) into Eq. (32) gives

$$-\frac{\rho'}{\bar{\rho}^2} = \frac{\rho}{\bar{\rho}^2}\left(\frac{f_A'}{\bar{\rho}_A} + \frac{f_B'}{\bar{\rho}_B} + \frac{f_C'}{\bar{\rho}_C}\right) - \left(\frac{\tilde{f}_A}{\bar{\rho}_A} + \frac{\tilde{f}_B}{\bar{\rho}_B} + \frac{\tilde{f}_C}{\bar{\rho}_C}\right)\left(\frac{p'}{\bar{p}} - \frac{\rho T'}{\bar{\rho}\tilde{T}}\right)$$

Combination of the last equation with Eq. (6) then gives

$$-\frac{\rho'}{\bar{\rho}} = \rho\left(\frac{f_A'}{\bar{\rho}_A} + \frac{f_B'}{\bar{\rho}_B} + \frac{f_C'}{\bar{\rho}_C}\right) - \left(\frac{p'}{\bar{p}} - \frac{\rho T'}{\bar{\rho}\tilde{T}}\right) \tag{34}$$

Eq. (34) is now used to replace ρ' in the enthalpic production term which is restated here as

$$\text{Enthalpic Generation} = -\overline{u_i'}\,\frac{\partial\bar{p}}{\partial x_i} = \frac{\overline{\rho' u_i'}}{\bar{\rho}}\,\frac{\partial\bar{p}}{\partial x_i}$$

Introduction of Eq. (34) yields

$$-\overline{u_i'}\,\frac{\partial\bar{p}}{\partial x_i} = \left[-\rho u_i'\left(\frac{f_A'}{\bar{\rho}_A} + \frac{f_B'}{\bar{\rho}_B} + \frac{f_C'}{\bar{\rho}_C}\right) + \frac{\overline{p' u_i'}}{\bar{p}} - \frac{\overline{\rho u_i' T'}}{\bar{\rho}\tilde{T}}\right]\frac{\partial\bar{p}}{\partial x_i}$$

Thus far, the treatment of the effects of density fluctuations has been exact. But now, approximations are made (or modelled) in the individual terms in the last expression. According to the eddy diffusivity model that is being used presently, Eq. (20) can be used to replace many of the terms in the expression. Hence,

$$-\overline{u_i'}\,\frac{\partial\bar{p}}{\partial x_i} = \left[\frac{\mu_t}{\sigma_{t,f}}\left(\frac{1}{\bar{\rho}_A}\frac{\partial\tilde{f}_A}{\partial x_i} + \frac{1}{\bar{\rho}_B}\frac{\partial\tilde{f}_B}{\partial x_i} + \frac{1}{\bar{\rho}_C}\frac{\partial\tilde{f}_C}{\partial x_i}\right) + \frac{\overline{p'u_i'}}{\bar{p}} + \frac{\mu_t}{\sigma_{t,h}}\,\frac{1}{\bar{\rho}\tilde{h}}\,\frac{\partial\tilde{h}}{\partial x_i}\right]\frac{\partial\bar{p}}{\partial x_i}$$

where in the last expression, the temperature has been replaced by the specific enthalpy. Earlier, it was argued that pressure fluctuations are negligible compared to the rest of the fluctuations; therefore, the term $\overline{p'u_i'}$ can be dropped. The final expression then becomes

$$-\overline{u_i'}\,\frac{\partial\bar{p}}{\partial x_i} = \left[\frac{\mu_t}{\sigma_{t,f}}\left(\frac{1}{\bar{\rho}_A}\frac{\partial\tilde{f}_A}{\partial x_i} + \frac{1}{\bar{\rho}_B}\frac{\partial\tilde{f}_B}{\partial x_i} + \frac{1}{\bar{\rho}_C}\frac{\partial\tilde{f}_C}{\partial x_i}\right) + \frac{\mu_t}{\sigma_{t,h}\bar{\rho}\tilde{h}}\,\frac{\partial\tilde{h}}{\partial x_i}\right]\frac{\partial\bar{p}}{\partial x_i} \tag{35}$$

So far, two different expressions, Eqs. (31) and (35), have been derived to represent the same term. It will be shown now that they are essentially equivalent. Consider Eq. (31); if the term pertaining to the rate of strain ε_{ij} is neglected, the expression becomes

$$-\overline{u_i'}\,\frac{\partial\bar{p}}{\partial x_i} = -\,\frac{C_3\mu_t}{\bar{\rho}^2}\,\frac{\partial\bar{\rho}}{\partial x_i}\,\frac{\partial\bar{p}}{\partial x_i}$$

Differentiation and manipulation of Eqs. (6) and (7) give

$$\frac{1}{\bar{\rho}^2}\frac{\partial\bar{\rho}}{\partial x_i} = -\left[\frac{1}{\bar{\rho}_A}\frac{\partial\tilde{f}_A}{\partial x_i} + \frac{1}{\bar{\rho}_B}\frac{\partial\tilde{f}_B}{\partial x_i} + \frac{1}{\bar{\rho}_C}\frac{\partial\tilde{f}_C}{\partial x_i}\right] + \frac{1}{\bar{\rho}\bar{p}}\frac{\partial\bar{p}}{\partial x_i} - \frac{1}{\bar{p}\tilde{T}}\frac{\partial\tilde{T}}{\partial x_i}$$

Therefore,

$$-\overline{u_i'}\frac{\partial\bar{p}}{\partial x_i} = C_3\mu_t\left[\frac{1}{\bar{\rho}_A}\frac{\partial\tilde{f}_A}{\partial x_i} + \frac{1}{\bar{\rho}_B}\frac{\partial\tilde{f}_B}{\partial x_i} + \frac{1}{\bar{\rho}_C}\frac{\partial\tilde{f}_C}{\partial x_i} - \frac{1}{\bar{\rho}\bar{p}}\frac{\partial\bar{p}}{\partial x_i} + \frac{1}{\bar{\rho}\tilde{h}}\frac{\partial\tilde{h}}{\partial x_i}\right]\frac{\partial\bar{p}}{\partial x_i}$$

The last expression is almost identical to Eq. (35); the extra term involving $\partial\bar{p}/\partial x_i$ is not obtained in Eq. (35) because of the neglect of the term $\overline{p'u_i'}$ in its derivation. It is clear that the two different approaches lead to almost identical expressions, which enhances the confidence in their correctness.

A final recommendation as to what form of the enthalpic generation term should assume may be put forward. Since the neglect of term ε_{ij} in Eq. (31) leads to an expression very similar to that in Eq. (35), hence, it may be neglected, leaving the expression

$$-\overline{u_i'}\frac{\partial\bar{p}}{\partial x_i} = -\frac{C_3\mu_t}{\bar{\rho}^2}\frac{\partial\bar{\rho}}{\partial x_i}\frac{\partial\bar{p}}{\partial x_i} \tag{36}$$

As Eq. (36) is simpler than Eq. (35), the former is recommended for use in the k-equation.

5. FINAL SET OF EQUATIONS

The final set of equations will now be summarized. Since molecular diffusion plays a trivial role in the large-scale mixing of the present problem, the terms expressing its effects have been dropped. The overbars and ∿ will be suppressed, because all the dependent variables are taken to be the mean value of the property solved for.

Continuity

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j) = 0 \tag{37}$$

Momentum

$$\frac{\partial}{\partial t} \rho u_i + \frac{\partial}{\partial x_j} (\rho u_j u_i) = - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \mu_t \varepsilon_{ij} - \frac{2}{3} \frac{\partial}{\partial x_i} \rho k \tag{38}$$

where

$$\varepsilon_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_n}{\partial x_n} \tag{39}$$

Energy

$$\frac{\partial}{\partial t} \rho E + \frac{\partial}{\partial x_j} \rho u_j (E + P/\rho) = \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_{t,h}} \frac{\partial h}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left[u_i \left(\mu_t \varepsilon_{ij} - \frac{2}{3} \delta_{ij} \rho k \right) + \frac{\mu_t}{\sigma_{t,k}} \frac{\partial k}{\partial x_j} \right] + Q \tag{40}$$

where

$$E \equiv e + \frac{1}{2} u_i u_i + k \tag{41}$$

Mass Fraction

$$\frac{\partial}{\partial t} \rho f_\alpha + \frac{\partial}{\partial x_j} (\rho u_j f_\alpha) = \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_{t,f}} \frac{\partial f_\alpha}{\partial x_j} \right) + S_\alpha \tag{42}$$

Turbulent Kinetic Energy

$$\frac{\partial}{\partial t} \rho k + \frac{\partial}{\partial x_j} (\rho u_j k) = \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_{t,k}} \frac{\partial k}{\partial x_j} \right) + G - \rho \varepsilon \tag{43}$$

where

$$G \equiv \left(\mu_t \varepsilon_{ij} - \frac{2}{3} \delta_{ij} k \rho \right) \frac{\partial u_i}{\partial x_j} - \frac{C_3 \mu_t}{\rho^2} \frac{\partial \rho}{\partial x_j} \frac{\partial p}{\partial x_i} \tag{44}$$

Dissipation of Turbulent Kinetic Energy

$$\frac{\partial}{\partial t} \rho \varepsilon + \frac{\partial}{\partial x_j} (\rho u_j \varepsilon) = \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_{t,\varepsilon}} \frac{\partial \varepsilon}{\partial x_j} \right) + C_1 G \frac{\varepsilon}{k} - C_2 \rho \frac{\varepsilon^2}{k} \tag{45}$$

Turbulent Viscosity

$$\mu_t = C_\mu \rho \frac{k^2}{\varepsilon}$$

This closes the set of equations.

Turbulence model constants C_1, C_2, C_μ, and the turbulent Prandtl numbers $\sigma_{t,h}$, $\sigma_{t,k}$, etc., have been derived for turbulent shear flows. Values for these constants that are normally recommended for such shear flows are given in Table 1. These values can be used as initial guesses for the present problem. However, one should be prepared to experiment with these values and to verify their validity for such Rayleigh-Taylor mixing problems by comparison with experimental data. A new constant C_3 has been introduced in the present document; it is roughly inversely proportional to the turbulence Prandtl number (compare Eqs. (36) and (37)). It should therefore lie between 0.7 to 1.5.

TABLE 1. VALUES OF CONSTANTS, AS DERIVED FOR SHEAR DOMINATED FLOWS

Constant	Value
C_1	1.44
C_2	1.92
C_3	0.7-1.5
C_μ	.09
$\sigma_{t,h}$	1.0
$\sigma_{t,k}$	1.0
$\sigma_{t,f}$	1.0
$\sigma_{t,\varepsilon}$	1.3

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APPENDIX A
EXPANSION OF THE GOVERNING EQUATIONS
FOR SPHERICALLY SYMMETRICAL FLOW

Eqs. (37) to (44) are expanded in this appendix in spherical coordinates assuming spherical symmetry of the flow.

Continuity

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \quad) = 0 \tag{A1}$$

Momentum

$$\frac{\partial}{\partial t} (\rho u) + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho u^2) = - \frac{\partial}{\partial r} \left(p + \frac{2}{3} \rho k\right) \tag{A2}$$

Energy

$$\frac{\partial}{\partial t} (\rho E) + \frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 \rho u\left(E + \frac{p}{\rho} + \frac{2}{3} k\right)\right] =$$

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 \left(\frac{\mu_t}{\sigma_{t,h}} \frac{\partial h}{\partial r} + \frac{\mu_t}{\sigma_{t,k}} \frac{\partial k}{\partial r}\right)\right] + Q \tag{A3}$$

where

$$E \equiv e + \frac{1}{2} u^2 + k$$

Mass Fraction

$$\frac{\partial}{\partial t} (\rho f_\alpha) + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho u f_\alpha) = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\mu_t}{\sigma_{t,f}} \frac{\partial f_\alpha}{\partial r}\right) + S_\alpha \tag{A4}$$

Turbulent Kinetic Energy

$$\frac{\partial}{\partial t}(\rho k) + \frac{1}{r^2}\frac{\partial}{\partial r^2}(r^2 \rho u k) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\mu_t}{\sigma_{t,k}} \frac{\partial k}{\partial r}\right) + G - \rho\varepsilon \quad \text{(A5)}$$

Dissipation of Turbulent Kinetic Energy

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 \rho u \varepsilon) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\mu_t}{\sigma_{t,\varepsilon}} \frac{\partial \varepsilon}{\partial r}\right) + C_1 G \frac{\varepsilon}{k} - C_2 \rho \frac{\varepsilon^2}{k} \quad \text{(A6)}$$

where

$$G \equiv -\frac{2}{3}\frac{\rho k}{r^2}\frac{\partial}{\partial r}(r^2 u) - \frac{C_3 \mu_t}{\rho^2}\frac{\partial \rho}{\partial r}\frac{\partial p}{\partial r}$$

The constants C_1, C_2, etc., were given in Table 1.

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